IUCLID

Data Set

Existing Chemical : ID: 61788-32-7 **CAS No.** : 61788-32-7

EINECS Name : Terphenyl, hydrogenated

EC No. : 262-967-7

TSCA Name : Terphenyl, hydrogenated

Producer related part

Company : Solutia Inc. Creation date : 17.03.2003

Substance related part

Company : Solutia Inc. Creation date : 17.03.2003

Status : Memo :

Printing date : 28.07.2003

Revision date :

Date of last update : 28.07.2003

Number of pages : 28

Chapter (profile) : Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile) : Reliability: without reliability, 1, 2, 3, 4

Flags (profile) : Flags: without flag, confidential, non confidential, WGK (DE), TALuft (DE),

Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1. General Information

ld 61788-32-7 **Date** 28.07.2003

1.0.1	0.1 APPLICANT AND COMPANY INFORMATION				
1.0.2	.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR				
1.0.3	IDENTITY OF RECIPIEN	vts			
404	DETAILS ON CATEGOR	DV/TEA/DLATE			
1.0.4	DETAILS ON CATEGO	RITIENPLATE			
1.1.0	SUBSTANCE IDENTIFIC	CATION			
Reli	ability	: (1) valid without restriction			
	06.2003	· ,			
1.1.1	GENERAL SUBSTANC	E INFORMATION			
	OLIVAL GODOTANO				
Pur	ity type	•			
Sub	stance type	: organic			
Phy Pur	sical status	: : > 98 - % v/v			
Col		. > 90 - 70 V/V			
Odour :		:			
Tes	t substance	: Commercial Grade of greater than 98% purity. Consists of approxim ately			
		40% Partially Hydrogenated Terphenyls (80-85%) and Quaterphenyls (15-20%).			
24.0	06.2003	2070).			
1.1.2	SPECTRA				
1.2	SYNONYMS AND TRAI	DENAMES			
1.3	IMPURITIES				
1.4	ADDITIVES				
1.5	5 TOTAL QUANTITY				
1.6.1	1.6.1 LABELLING				

1. General Information

ld 61788-32-7 **Date** 28.07.2003

1.6.2	CLASSIFICATION
1.6.3	PACKAGING
1.7	USE PATTERN
1.7	OSEFATIENT
1.7.1	DETAILED USE PATTERN
1.7.2	METHODS OF MANUFACTURE
1.8	REGULATORY MEASURES
1.8.1	OCCUPATIONAL EXPOSURE LIMIT VALUES
1.8.2	ACCEPTABLE RESIDUES LEVELS
1.8.3	WATER POLLUTION
1.8.4	MAJOR ACCIDENT HAZARDS
1.8.5	AIR POLLUTION
1.0.5	AIR POLLOTION
1.8.6	LISTINGS E.G. CHEMICAL INVENTORIES
1.9.1	DEGRADATION/TRANSFORMATION PRODUCTS
1.9.2	COMPONENTS
1.10	SOURCE OF EXPOSURE
4.44	ADDITIONAL DEMARKS
1.11	ADDITIONAL REMARKS
1.12	LAST LITERATURE SEARCH

1. General Information

ld 61788-32-7 **Date** 28.07.2003

1.13 REVIEWS

2. Physico-Chemical Data

ld 61788-32-7 **Date** 28.07.2003

2.1 MELTING POINT

Value : -32 - °C

Sublimation

Method

Year : 2003

GLP

Test substance: as prescribed by 1.1 - 1.4

Result: As this material is a liquid at room temperature, the mp has been

expressed as the pour point.

Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint

24.06.2003

2.2 BOILING POINT

Value : 359 - °C at

Decomposition

Method

Year : 2003

GLP

Test substance : as prescribed by 1.1 - 1.4

Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint

24.06.2003 (1)

2.3 DENSITY

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value : .002666 - hPa at 25 °C

Decomposition : Method :

Year : 1985 **GLP** : no data

Test substance : as prescribed by 1.1 - 1.4

Method : Gas saturation technique.

Remark : Reported as 0.002 @ mm Hg 25 deg C.

Test substance : MXP-2020, a precommercial sample of THERMINOL 66 of essentially

same purity of approx. 98%.

Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint

24.07.2003 (2)

2.5 PARTITION COEFFICIENT

2. Physico-Chemical Data

ld 61788-32-7 **Date** 28.07.2003

Partition coefficient : octanol-water Log pow : 6.13 - at 23 °C

pH value : Method :

Year : 1977 **GLP** : no

Test substance: as prescribed by 1.1 - 1.4

Method : Partition coefficient was determined via a direct partition experiment. At

least two concentrations of the test substance were prepared in 100 ml of n-octanol. The n-octanol test solutions were combined with 500 ml purified water in a 1-l glass bottle at room temperature (ca. 25 deg. C) and shaken for 48 hours. Shaken mixtures were allowed to separate for 1 week in the dark. Concentrations of the test substance in each phase were determined by gas chromatography with dual flame-ionization detectors (GC -FID/FID). The partition coefficient (P) was calculated using the following equation:

P = Co/Cw

where Co and Cw are the concentrations of the test substance in n-octanol

and water, respectively.

Result: Reported as 1.36x10E6.

Test substance : Santosol 340

Reliability : (2) valid with restrictions

Flag : Critical study for SIDS endpoint

24.07.2003 (3)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in : Water

Value : < .06 - mg/l at 23 °C

pH value :

concentration : at °C

Temperature effects

Examine different pol.

pKa : at 25 °C

Description : Stable :

Stable Deg. product

Method : OECD Guide-line 105

Year : 1995 GLP : no data

Test substance : as prescribed by 1.1 - 1.4

Remark : Value cited was maximum value, as the methodology would not allow

attempts for detection at even lower levels.

Test substance: Santotherm 66

Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint

24.07.2003 (4)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

2. Physico-Chemical Data

ld 61788-32-7 **Date** 28.07.2003

2.8	AUTO FLAMMABILITY
2.9	FLAMMABILITY
2.10	EXPLOSIVE PROPERTIES
2.11	OXIDIZING PROPERTIES
2.12	DISSOCIATION CONSTANT
2.13	VISCOSITY
2.14	ADDITIONAL REMARKS

3. Environmental Fate and Pathways

ld 61788-32-7 **Date** 28.07.2003

3.1.1 PHOTODEGRADATION

Deg. product :

Method : other (measured)

Year : 1982 GLP : no data Test substance : other TS

Method : Direct analysis of photodegradation in sunlight. A 50 mg/L aqueous

concentration using acetonitrile solvent was added to duplicate quartz tubes, sealed and exposed to sunlight (> 100 hrs over 15 day test period) at ave. temp. of 62 deg. F. Test sample was measured at intervals of 0, 2, 5, 9 and 15 days after exposure. Darkened tubes were also analyzed and amount of degradation subtracted from light-exposed tubes to define the

degree of photolysis. Analysis conducted using GC-FID.

Result : T 1/2 = 86 days

Test substance : MXP-2020, an precommercial sample of THERMINOL 66 of similar purity

of approx. 98%.

Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint

28.07.2003 (5)

3.1.2 STABILITY IN WATER

Remark: Test material is not susceptible to hydrolysis.

28.07.2003

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type : fugacity model level III

Media

Air : .229 % (Fugacity Model Level I)

Water : 3.57 % (Fugacity Model Level I)

Soil : 27.5 % (Fugacity Model Level I)

Biota : % (Fugacity Model Level II/III)

Soil : 68.7 % (Fugacity Model Level II/III)

Method : other:Calculation based on EPISUITE

Year : 2003

Method : Level III fugacity based model, EPISUITE 3.10. Default values were

assumed for environmental compartment descriptions, dimensions and properties, advective and dispersive properties. Chemical-specific modeling parameters as calculated by the model were: molecular weight= 242.41 g/mol, vapor pressure = 0.00012 hPa at 25 deg. C, log Kow = 7.63,

3. Environmental Fate and Pathways

ld 61788-32-7 **Date** 28.07.2003

melting point = 77.77 deg. C. and a Henry's Law constant of 0.00292 atm-m3/mol. Half-lives calculated by the model based on the properties of the test substance were: air half-life = 8.29 hr, water and soil half-lives = 900 hr, and sediment half-life = 3600 hr. Emissions were assumed to be equal

to air, water, and soil.

Test substance : A representative structure of 1,3-Dicyclohexyl benzene (a major

component of Partially Hydrogenated Terphenyls) with a SMILES notation

of C(CCCC3)(C3)c(cccc1(C(CCCC2)C2))c1.

Reliability : (2) valid with restrictions

Flag : Critical study for SIDS endpoint

28.07.2003 (6)

3.3.2 DISTRIBUTION

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Type : aerobic

Inoculum : other: municipal sewage treatment plant

Concentration : 10 g/l related to Test substance

related to

Contact time : 9 month

Degradation : 35 - 1 (±8.6) % after 24 hour(s)

Result

Deg. product

Method : other: Semi-Continuous Activated Sludge (SCAS)

Year : 1971 **GLP** : no

Test substance: as prescribed by 1.1 - 1.4

Method : 9 month SCAS test generally consistent with OECD guideline 302, 4 test

periods of 4 to 29 days, 24-h cycle of draw and fill, weekly analyses of parent material using UV absorbance, while metabolites were quantified using GC-FID, 10 mg test material was added per cycle, activated sludge mixed liquor from municipal sewage treatment plant was inocula, a series

of 3 hexane off-gas scrubbers were used to catch volatiles.

Result : For time period 1, mean and 95% CI disappearance rate was 19.5 +/-

20.8%, for period 2 it was 55.0 + -12.9%, for period 3 it was 25.0 + -81.2% and for period 4 it was 48.6 + -6.9%. Overall mean daily disappearance rate was 35.1 + -8.6%. GC analyses showed that the several peaks that make up the test material degraded at varying levels. No volatile losses

were reported.

Test substance: HB-40

Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint

11.07.2003 (7)

Type : aerobic

Inoculum : other: Meramec River water

Contact time

Degradation : $68 - (\pm) \%$ after 50 day(s)

Result

Deg. product

Method : other: River -Die Away test

Year : 1971 **GLP** : no

9/28

3. Environmental Fate and Pathways

ld 61788-32-7 **Date** 28.07.2003

Test substance: as prescribed by 1.1 - 1.4

Method : River water was obtained from the Meramec River near St. Louis, Missouri,

USA. Settled water (2 days) was added (200 mL) to 16-oz. wide-mouth bottles. Distilled water controls (with test substance) were prepared similarly to assess sorption to glass and volatilization. Test material was added in 5 microliter volumes prepared with 4% (W/V) ethanol. Bottles were sealed with foil-lined caps and stored at room temperature in the dark for up to 50 days. A positive control (LAS Peferance #2, Dedecape 1)

for up to 50 days. A positive control (LAS Reference #2 - Dodecene-1) was prepared similarly and used to verify the biological activity. Periodically, chemical analyses were made by sacrificing a bottle containing test material and a control. Three 50-mL aliquots of hexane were injected into the bottle, the bottle vigorously shaken, and the phases allowed to separate. The three portions of hexane were collected,

concentrated to 10 mL using a Kudema-Danish concentrater, transferred to a 10 mL cell and the UV absorption determined. Recoveries of spiked

samples for the test substance were 91.6%.

Result : Losses from the distilled water control were 13%. Test material was

reduced by 68% in 21 days and by 81% (net loss of 68%) in 50 days.

Test substance : HB-4

Reliability : (2) valid with restrictions

Supplemental information which indicates considerable biological

breakdown in the environment.

11.07.2003 (7)

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type : static

Species: Pimephales promelas (Fish, fresh water)

 Exposure period
 : 96 hour(s)

 Unit
 : mg/l

 LC50
 : > .06

 Limit test
 : yes

 Analytical monitoring
 : no

Method : other: US EPA 660/3-75-009

Year : 1979 **GLP** : yes

Test substance: as prescribed by 1.1 - 1.4

Method : This study followed US EPA guideline 660/3-75-009. 1975. Committee on

Methods for Toxicity Tests with Aquatic Organisms. Fathead minnows were obtained from a fish hatchery, held in culture tanks for two weeks under 16 hrs light, 8 hrs dark. Fish were fed commercial fish food until 48 hr before the test. Fish had a mean weight and length of 0.46 g and 30.4 mm, respectively. Static bioassay was performed in a 40 L glass aquaria containing 30 L of laboratory well water and 10 (ten) fish per concentration. Antimycin a was used as a positive control. Water quality of test dilution at test initiation was: DO 9.3 mg/L, pH 7.8-8.2, total hardness of 255 mg/L CaCO3, total alkalinity of 368 mg/L CaCO3. Test water was maintained at 22 +/- 1 deg. C in a water bath. Fish were held without food for 48 hrs before testing and were not fed during the test. Based on finding no toxicity at 1000 mg/L in a range-find test, a definitive test was conducted at 1,000 mg/L nominal test material. A test concentration was prepared by adding test material directly to the test vessel; no meaurements of test material were taken during the test. An oily film was observed in the test vessels during the study. Across all test vessels, DO varied between 5.2 to 8.5 mg/L, pH ranged from 7.3-8.3, temperature remained close to 22 deg.

Ċ.

Result : No control mortalities were observed and only 10% deaths were seen in the 1000 mg/L Limit Test dose after 96 hours of testing. Thus the 96-h

the 1000 mg/L Limit Test dose after 96 hours of testing. Thus the 96-h LC50 was > 1000 mg/L nominal. As the water solubility of the test agent is

less than 0.06 mg/L., then the LC50 correctly stated is > 0.06 mg/L.

Test substance : Therminol 66

Reliability : (2) valid with restrictions

While the nominal dose level used in this study well exceeded the water solubility of Therm inol 66, it can reasonably be concluded that the 96-h EC50 is in excess of the water solubility limit, as the nominal concentration

proved to produce only limited (10% deaths) toxicity.

Flag : Critical study for SIDS endpoint

28.07.2003 (8)

Type : static

Species : Salmo gairdneri (Fish, estuary, fresh water)

 Exposure period
 : 96 hour(s)

 Unit
 : mg/l

 LC50
 : > .06

 Limit test
 : yes

 Analytical monitoring
 : no

Method : other: US EPA 660/3-75-009

Year : 1979 **GLP** : ves

Test substance: as prescribed by 1.1 - 1.4

Method : This study followed US EPA guideline 660/3-75-009. 1975. Committee on

Methods for Toxicity Tests with Aquatic Organisms. Rainbow trout were obtained from a fish hatchery, held in culture tanks for two weeks under 16 hrs light, 8 hrs dark. Fish were fed commercial fish food until 48 hr before the test. Fish had a mean weight and length of 1.02 g and 39.1 mm, respectively. Static bioassay was performed in a 5 gal, glass aguaria containing 15 L of laboratory well water. Ten (10) fish per test concentration level were used. Antimycin A was tested as a positive control. Water quality of test dilution at test initiation was: DO 8.9 mg/L, pH 7.8, total hardness of 240 mg/L CaCO3, total alkalinity of 360 mg/L CaCO3. Test water was maintained at 12 +/- 1 deg. C in a water bath. Fish were held without food for 48 hrs before testing and were not fed during the test. Based on finding no toxicity at 1000 mg/L in a range-find test, a definitive test was conducted at 1,000 mg/L nominal test material. A test concentration was prepared by adding test material directly to the test vessel; no meaurements of test material were taken during the test. An oily film was observed in the test vessels during the study. Across all test vessels, DO varied between 5.8 to 7.3 mg/L, pH ranged from 7.3-8.3, temperature remained at 12 deg. C.

Reliability : (2) valid with restrictions

Provided as Supplemental information. While the nominal dose level used in this study well exceeded the water solubility of Therminol 66, it is reasonable conclude that the 96-h EC50 is in excess of the water solubility limit (0.06 mg/L), as the nominal concentration proved to produce only

limited (10% deaths) toxicity.

28.07.2003 (9)

Type : other

Species : other: calculated
Exposure period : 96 hour(s)
Unit : mg/l

LC50 : = .00092 - calculated

Method : other: calculation based on ECOSAR

Year : 2003 GLP : no Test substance : other TS

Method : 96-Hr Fish LC50 calculation using ECOSAR, from the USEPA. Value was

calculated using a calculated log Kow of 7.63. The SAR for neutral

organics was employed.

Remark : Provided as Supplemental Information to this HPV data package.

Test substance : A representative structure of 1,3-Dicyclohexyl benzene (a major

component of Partially Hydrogenated Terphenyls) with a SMILES notation

of C(CCC3)(C3)c(cccc1(C(CCCC2)C2))c1.

28.07.2003 (10)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type : static

Species : Daphnia magna (Crustacea)

Exposure period : 48 hour(s)
Unit : mg/l

NOEC : >= 1.34 - measured/nominal **EC50** : >= 1.34 - measured/nominal

Limit Test : yes Analytical monitoring : yes

Method : OECD Guide-line 202

Year : 1996
GLP : yes
Test substance : other TS

Method

: Twenty < 24-h old D. magna Straus were tested at 20 +/- 1 deg. C in a series of four replicates per test concentration. The Limit Test was conducted at 1.34 mg/L and included clean water and solvent (ethoxylated triglyceride at 150 mg/L) controls. Stock solutions had a few white dustlooking particles floating on their surface. Tests were conducted using reconstituted distilled water. Water was reconstituted with CaCl2. MgSO4. NaHCO3 and KCl. At test initiation, the pH was 7.97. DO was at 23.8% of saturation, specific conductance was at 680 micro-siemens, hardness was 262 mg/L, alkalinity was 34 mg/L. Test concentrations were measured using HPLC. Daphnids were not fed during the test. Tests were conducted in 1 fluid ounce plastic cups containing 25 mL of solution. Dissolved oxygen, temperature and pH were monitored at the beginning and end of the test. At test initiation, the test substance concentration was 1.34 mg/L and at 28 hr it was 1.29 mg/L. A photoperiod was not specified in the report. However, as this study was conducted in late July/early August in St. Louis Mo. the average photoperiod in that location is approximately 16h light,8-h dark.

Result

Limit Test 48-h EC50 = >1.34 mg/L; 24-h EC50 > 1.34 mg/L. NOEC => 1.34 mg/L. There were no immobilizations reported in either control or in vessels with test substance at either 24 or 48 hrs. At test initiation, pH ranged from 7.96 to 8.03, DO ranged from 17.3 to 23.4% of saturation and temperature ranged from 22 to 23 deg. C. At 48 hrs, pH ranged from 7.77 to 8.02, DO ranged from 20.1 to 22.7% of saturation, and temperature ranged from 20.4 to 21.6 deg. C.

Test substance : THERMINOL 66

Reliability : (1) valid without restriction **Flag** : Critical study for SIDS endpoint

24.07.2003 (11)

Type : static

Species : Daphnia magna (Crustacea)

 Exposure period
 : 48 hour(s)

 Unit
 : mg/l

 NOEC
 : < .056 -</td>

 EC50
 : = .1

 Method
 : other

 Year
 : 1979

 GLP
 : ves

Test substance: as prescribed by 1.1 - 1.4

Method

Followed guidance according to EPA 660/3-75-009. Ten < 24-h old D. magna Straus were tested at 20 +/- deg. C. in a series of two replicates per test concentration. Test concentrations were 0.056 (level of solubility), 0.10, 0.18, 0.32 and 0.56 mg/L, plus clean water and solvent (acetone) controls. Tests were conducted using well water from Columbia, MO. Concentrations were not measured. Daphnids were not fed.

Tests were conducted in 250-mL beakers containing 200 mL of solution. Dissolved oxygen was monitored to ensure the concentration did not fall below 2 mg/L before the end of the test. Water quality was measured for dissolved oxygen, pH, ammonia, and temperature and no significant changes were observed in any parameter during the test. The estimated EC50 and 95% confidence limits were determined using EPA statistical procedures (probit analysis).

Remark Result Supplemental information

: 48-h EC50 (95% CL) = 0.10 (0.075-0.13) mg/L; 24-h EC50 (95% CL) = 0.70 (0.49-1.0); NOEC = < 0.056 mg/L.; At 24-h, there were no mortalities in controls or the lower two test concentrations. Clumping of daphnids was observed at the highest 3 concentrations. At 48-h, there were no mortalities (0/10; 0/10) in controls. There were partial mortalities in the lower three test concentrations [2/10;2/10 @ 0.056 mg/L; 4/10,5/10 @ 0.10 mg/L;8/10, 10/10 @ 0.18 mg/L]and 100% mortality in the highest two (0.32

13/28

& 0.56 mg/L) concentrations. Mortalities followed a dose-response pattern.

Test substance: Therminol 66

Reliability : (2) valid with restrictions

11.07.2003 (12)

Type : other: Calculation

Species : Daphnia magna (Crustacea)

Exposure period : 48 hour(s)
Unit : mg/l

EC50 : = .00145 - calculated

Method : other: calculation using ECOSAR

Year : 2003 GLP : no Test substance : other TS

Method : 48-Hr Daphnia LC50 calculation using ECOSAR, from the USEPA. Value

was calculated using a calculated log Kow of 7.63. The SAR for neutral

organics was employed.

Remark : Provided as Supplemental Information to this HPV data package.

Test substance : A representative structure of 1,3-Dicyclohexyl benzene (a major

component of Partially Hydrogenated Terphenyls) with a SMILES notation

of C(CCCC3)(C3)c(cccc1(C(CCCC2)C2))c1.

28.07.2003 (10)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species : Selenastrum capricornutum (Algae)
Endpoint : other: chlorophyl a, cell number

 Exposure period
 : 96 hour(s)

 Unit
 : mg/l

 EC50 (chlorophyl a)
 : > .06

 EC50 (cell number)
 : > .06

Limit test

Analytical monitoring : no

Method : other: US EPA, 1971.

Year : 1979 GLP : no data

Test substance : as prescribed by 1.1 - 1.4

Method : The study followed methods outlined in USEPA, 1971. Algal Assay

Procedure: Bottle Test. National Eutrophication Research Program. Pacific Northwest Water Laboratory, Corvallis, OR. Cultures were incubated at 24

+/- deg. C under 4000 lux illumination during a 24-h/d photoperiod.

Triplicate culture flasks were employed for each of the test concentrations and controls used. Nominal test concentrations were 10, 32, 56, 100 and

320 mg/L. Both clean water and solvent controls were included. Dimethylformamide (DMF) was used as a cosolvent (0.05 mL per test flask). Test material was dissolved in DMG and directly added to the test vessels. Initial cell counts were ~ 20,000 cells/mL. chlorophyll a was measured using a Turner Model 111 fluorometer. Cell counts were made using a hemacytometer and a Zeiss Standard 14 compound microscope. Specifics of the culture medium were not provided other than stating that test medium was based on USEPA guidance. Results were analyzed using the Student's t test. PH was maintained between 7.2 and 7.4 during

the test.

Result : Chlorophyll a

96-h EC50 (95% CI) = 44 (1-1586) mg/L. 24-h EC50 (95% CI) = >320 mg/L 48-h EC50 (95% CI) = >320 mg/L 72-h EC50 (95% CI) = >100 < 320 mg/L.

ld 61788-32-7 4. Ecotoxicity

Date 28.07.2003

Cell number

96-h EC50 (95% CI) = 56 (4-743) mg/L.

As the water solubility of THERMINOL 66 is less than 0.06 mg/L, this level was exceeded in both phases of this study. However, as there were no toxic effects observed at the lowest dose tested, it can be concluded that

the EC50 > 0.06.

Test substance : Therminol 66

Reliability (2) valid with restrictions

> All test levels exceeded the water solubility limit of Therminol 66 of less than 0.06 mg/L. However, the lowest dose levels in this study did not produce a treatment-related effect. Thus, it can be concluded that no effects were seen up to the level of water solubility for this material.

Critical study for SIDS endpoint Flag

28.07.2003 (13)

Species other algae

Endpoint other: calculation for green algae

Exposure period 96 hour(s) Unit : mg/l

EC50 = .00125 - calculated

Method other: calculation based on ECOSAR

Year 2003 **GLP** nο Test substance other TS

Method : 96-Hr Algae LC50 calculation using ECOSAR, from the USEPA. Value was

calculated using a calculated log Kow of 7.63. The SAR for neutral

organics was employed.

Remark Provided as Supplemental Information to this HPV Package. Test substance A representative structure of 1,3 -Dicyclohexyl benzene (a major

component of Partially Hydrogenated Terphenyls) with a SMILES notation

of C(CCC3)(C3)c(cccc1(C(CCCC2)C2))c1.

28.07.2003 (10)

TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4. Ecotoxicity

ld 61788-32-7 **Date** 28.07.2003

- 4.7 BIOLOGICAL EFFECTS MONITORING
- 4.8 BIOTRANSFORMATION AND KINETICS
- 4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

Type : other: Limit Test
Value : > 10000 - mg/kg bw

Species : rat

Strain : Sprague-Dawley
Sex : male/female

Number of animals : 10

Vehicle

Doses : 10,000 mg/kg

Method : OECD Guide-line 401 "Acute Oral Toxicity"

Year : 1979 **GLP** : yes

Test substance : as prescribed by 1.1 - 1.4

Method : A single group of 5 male and 5 female fasted SD rats were administered

10,000 mg/kg test material via gavage and observed for 15 days. Twice daily examinations were made for mortality and signs of toxicity. Body weights were recorded on the first day of testing and weekly thereafter. Food and water were given ad libitum. Temperature, humidity and light cycle were controled. At the end of the study, all survivors were given a full

necropsy.

Result : No deaths occurred at the single dosage level tested of 10,000 mg/kg.

Signs of toxicity included: hypoactivity, diarrhea and feces - and urine-

stained fur. All animals were normal at necropsy.

Test substance: Commercial grade HB-40 of > 98% purity.

Reliability : (1) valid without restriction **Flag** : Critical study for SIDS endpoint

24.06.2003 (14)

Type : other: Limit Test
Value : >24000 - mg/kg bw

Species : rat

Strain : Fischer 344
Sex : female

Number of animals

Vehicle: other: undilutedDoses: no data available

Method : other Year : 1979 GLP : no

Test substance : as prescribed by 1.1 - 1.4

Method : Female F344 rats, 12-14 weeks old, were fasted overnight and then dosed

by gavage with undiluted test material. No dosage exceeded 24 g/kg bw. Five rats per treatment group were tested using dosages spaced at 0.1 log increments. Animals were maintained at 20 +/- 2 deg. C, 12-hr light:dark cycle and had water and food provided ad libitum. Daily observations for clinical signs were taken throughout the 14-day test period; body weights were recorded prestudy and weekly thereafter. Gross pathological examinations were carried out on selected animals which survived the highest dose tested. As this study resulted in a Limit Test, no LD50 calculation, using the method of Deichmann and LeBlanc, was made.

Result : LD50 value was determined to be above the highest dose tested of 24,000

mg/kg. Other than diarrhea during the first 24-hrs, no other clinical signs of

toxicity were reported. No evidence of gross pathological effects were

reported.

Test substance: Test material was referenced as commercial grade THERMINOL 66,

obtained from Monsanto Co.

Reliability : (2) valid with restrictions

This information is supplied as Supplemental to a previously reported Limit

Test by the oral route for THERMINOL 66.

26.06.2003 (15)

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

5.2.2 EYE IRRITATION

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

Type : Sub-chronic

Species : rat

Sex : male/female
Strain : Sprague-Dawley
Route of admin. : oral feed
Exposure period : 91 days

Frequency of treatm. : daily
Post exposure period : none

Doses : 50, 200, 2000 ppm

Control group : yes

NOAEL : >= 200 - ppm **LOAEL** : >= 2000 - ppm

Method : OECD Guide-line 408 "Subchronic Oral Toxicity - Rodent: 90-day Study"

Year : 1984 **GLP** : yes

Test substance : as prescribed by 1.1 - 1.4

Method : Groups of 12 male and 12 female SD rats (approx. 4 wks old) were

administered a diet admixed directly with test material for 91 days. Levels of test material were verified during weekly diet analysis. All rats were examined for morbidity and mortality twice daily. Body weights and food consumption were measured weekly, and detailed signs of toxicity recorded. Humidity, temperature and lighting were controled. Clinical pathology for the following indices were measured for 10 rats/sex/group after 1 and again after 3 months on test: Hematology - HCT, HGB, RBC, WBC, Platelets, erythrocyte morphology and differ. leukocytes; Serum Chemistry - Ca, In. Phos, CL, Na, K, GLU, ALT, AST, BUN, Albumin, globulin, T. Prot., Creat., T. Bili and GGTP. An ophthalmoscopic

18/28

examination was given to all rats prior to study start and at study term. At the end of the study, all rats were given a necropsy and organ weights and body:organ weight ratios recorded for: brain, kidney, liver, testes and adrenals. Histopathological examination of a full set of tissues and organs, including ovaries, testes, adrenals, aorta, bone, marrow, femur, brain, esophagus, eyes, exorbital lacrimal gland, heart, intestines (6 sections), kidneys, liver, lungs, lymph nodes, mammary gland, uterus, pancreas, pituitary, prostate, salivary gland, seminal vesicles, skel. muscle, skin, spinal cord, nerve, spleen, stomach, thymus, thyroid/parathyroid, trachea, epididymides and all gross lesions were given to all rats in the control and high dose group. Livers, Lungs and kidneys from all mid and low dose animals were also examined microscopically. Statistical analysis of body weights, food consumption, growth rates, clinical pathology, organ weights and ratios were performed using Leven's Test for homogeneity and ANOVA followed by Terpstra-Jonckheere test and Dunnett's test for groupwise comparison.

Remark

: Based on food consumption and body weight data conversion factors, the dosages of test articles employed in this study were approximately 150, 15 and 3.5 mg/kg/d.

Result

: The NOAEL for this study is considered to be 200 ppm.

The following treatment-related effects seen at 2000 ppm were minimal in nature: small decreases in body weight in males (2.7%) and females (6-7%). Small but statistically significant decreases in hemoglobin, hematocrit and erythrocyte count were observed in high dose males, but not females, at the 1 month interval, but were no longer statistically significant at study termination. A statistical increase in platelet counts was seen in this study group at both the 1 and 3 month interval.

Cholesterol and albumin were elevated in high dose males after 3 months (cholesterol also after 1 mo.). Both males and females exhibited increased absolute kidney and liver weight increases as well as corresponding increased organ/body and organ/brain weight ratios. Microscopic evaluation resulted in no morphological evidence of a direct toxicopathologic effect of treatment. High dose males, but not females, had an increased incidence (but similar level of severity) of a spontaneously occurring regenerative renal lesion also present in control male rats. The pathological significance of this finding was deemed unclear. No treatment-related effects were seen on male or female reproductive organs.

Test substance: Therminol 66

Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint

11.07.2003 (16)

5.5 GENETIC TOXICITY 'IN VITRO'

Type : Ames test

System of testing : Salmonella typhimurium tester strains TA 1535, 1537, 1538, 98 and 100

Test concentration : 1 to 10,000 ug/plate

Cycotoxic concentr. : not reported; none apparently seen up to highest dose tested

Metabolic activation: with and without

Result : negative

Method : other: Ames et al. 1975. Mutat. Res. 31:347-364.

Year : 1979 **GLP** : no

Test substance : as prescribed by 1.1 - 1.4

Method : Method of testing and evaluation used the procedures described in Ames

et al, 1975, Mutat. Res. 31:347-354. Test samples diluted in dimethyl sulfoxide were prepared to give final concentrations ranging from 1 to 10,000 ug/plate in 0.1 ml. Negative and positive controls (MNNG, 2-AAF

abd 9-AA) were used. Each of 5 Salmonella tester strains, TA1535, 1537, 1538, 98 and 100 were tested in replicate plates with and without inclusion of liver homogenates from Arochlor 1254-treated male rats as the

activation system.

Result : No significant mutagenic activity seen in any of the Salmonella tester

strains used, with or without metabolic activation.

Test substance : Commercial grade sample of THERMINOL 66, obtained from Monsanto

Co.

Reliability : (2) valid with restrictions

No data shown in peer-reviewed publication; however, raw data is on file at

the Environmental Mutagen Information Center, Oak Ridge, Tenn.

Flag : Critical study for SIDS endpoint

24.07.2003 (15)

Type : Ames test

System of testing : Salmonella tester strains TA 1535, 1537, 98, 100

Test concentration : 10, 3, 1, 0.2, 0.04, 0.01 ul/plate

Cycotoxic concentr. : > 100 ul/plate

Metabolic activation : with and without

Result : negative

Method : OECD Guide-line 471

Year : 1978 **GLP** : yes

Test substance: as prescribed by 1.1 - 1.4

Method : Method used was plate incorporation assay based on Ames test methods

consistent with OECD 471. A single test was run in triplicate at each dosage both with and without metabolic activation. The S-9 liver

homogenates were prepared from male rats and given Arochlor 1254. All tester strains were obtained from Dr. B. Ames. Sterile DMSO was used as the solvent and a solvent control was employed of 20 uL/plate DMSO. Positive controls used were: 2-aminoanthracene. NaNo2 and 2-

Positive controls used were: 2-aminoanthracene, NaNo2 and 2-nitrofluorene. A positive response was determined upon observation of a statistically significant dose-response increase in revertant colonies. Bartlett's test was used for pairwise comparison to controls and dose response determined using regression analysis for log-log straight lines; P<0.01 was used.A spot test was also conducted using a single dosage of 50 ul/plate with and without S-9. A toxicity test was run using TA-100 with and without S-9 at dosages of 100, 30, 10, 1, 0.3, and 0.1 ul/plate.

Result : No mutagenic changes were observed in any of the four tester strains

used, with or without metabolic activation. No effects on background lawn were observed up to 100 ul/plate. No treatment-related mutagenic effects were observed in the Spot test, with or without metabolic activation, in any

of the four tester strains.

Test substance : HB-40

Reliability : (2) valid with restrictions

Study limited to 4 of 5 Salmonella tester strains called for in test guidelines and used only a single test without confirmation. Highest test dose was below limit of toxicity. However, study confirms results of previously

reported Salmonella test used to fulfill this HPV endpoint.

11.07.2003 (17)

5.6 GENETIC TOXICITY 'IN VIVO'

Type : Cytogenetic assay

Species : rat

Sex : male/female
Strain : Fischer 344

Route of admin. : i.p. Exposure period : 24 hours

Doses : 250, 1250, 2500 mg/kg

Result : negative

Method : OECD Guide-line 475 "Genetic Toxicology: In vivo Mammalian Bone

Marrow Cytogenetic Test - Chromosomal Analysis"

Year : 1986 **GLP** : yes

Test substance: as prescribed by 1.1 - 1.4

Method : Dose levels selected based on both a range-find study followed by a pilot

study where severe signs of toxicity and deaths (8/10) were seen at 5000 mg/kg test agent, the highest dose used in this study design. Six Fischer-344 rats/sex/time period were administered test agent in corn oil by intraperitoneal injection. Metaphase cells were collected from rat bone marrow (femur) at harvest times of 6, 12 and 24 hrs after treatment. Colchicine was administered 2 hr prior to sacrifice to arrest cells in cmetaphase. Marrow was exposed to hypotonic solution and fixed, cells and slides prepared and stained. All slides were coded before reading. Positive (Triethylene melamine) and negative (corn oil and untreated) controls were used for comparative purposes. Mitotic index was calculated based on counting of at least 1000 slides and chromosomal aberrations evaluated from at least 60 slides per animal per time point from the untreated control groups (male and female) and the 2,500 mg/kg test groups. All breaks, deletions, translocations and other changes were recorded. Mitotic Index, % chromosomally aberrant cells and frequency of chromosomal aberrations per cell were compared between treated vs control groups

Result: No significant differences in % chromosomally aberrant cells or frequency

of chromosomal aberrations/cell were observed between the negative control group and any of the test article treated groups at any of the three time points investigated. The positive control performed as expected. No

evidence of cytotoxicity was observed at any test level.

using ANOVA and Dunnett's test. P < 0.05 was used.

Test substance : Therminol 66

Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint

24.07.2003 (18)

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

Type : Two generation study

Species : ra

Sex: male/femaleStrain: Sprague-Dawley

Route of admin. : oral feed

Exposure period : F0 & F1 Adults-premating through litter weaning (Fo) and postweaning (F1)

Frequency of treatm. : daily

Premating exposure period

 Male
 :
 FO- 14 weeks; F1- 18 weeks

 Female
 :
 FO- 14 weeks; F1- 18 weeks

 Duration of test
 :
 FO WF - 167d; F1 W/F- 219d

No. of generation : 2

studies

Doses : 30, 100, 300, 1000 ppm Control group : yes, concurrent vehicle

NOAEL parental : = 1000 - ppm NOAEL F1 offspring : = 1000 - ppm NOAEL F2 offspring : = 1000 - ppm

21/28

Method : OECD Guide-line 416 "Two-generation Reproduction Toxicity Study"

Year : 1991 **GLP** : yes

Test substance : as prescribed by 1.1 - 1.4

Method

Test material was administered in the diet to groups of 30M and 30F rats of the F0 and F1 generations during a premating (70 days) growth period, and through the ensuing mating, gestation and lactation intervals (1 litter/generation) until day 21 post-partum. Dietary concentrations were analyzed by GC-FID weekly (all test levels first 4 weeks of the study, then one dose level weekly thereafter) to establish stability, homogeneity of mixing and target concentration accuracy. Body weights were recorded weekly for F0 and F1M. For F0 and F1 F wts were recorded weekly through the growth period and up to mating, then resumed after mating until sacrifice. Food consumption was recorded weekly for F0 and F1 M from study start up to mating, then resumed after mating through study term. Food consumption for adult females F0 and F1 was recorded weekly through the growth period and again after weaning of litters. Cageside observations for morbidity and mortality were made weekly, as well as daily observations of clinical signs. Temperature, humidity and light-dark cycles were controlled. F0 and F1 adults were sacrificed following weaning of their respective litters and given a gross postmortem examination. Reproductive tissues (testes, epididymides, seminal vesicles, uterus, vagina, mammary glands, prostate, ovaries) and selected other tissues (liver, pituitary, skin, and all gross lesions) were evaluated histopathologically for all control and high dose animals. Pups delivered to F0 and F1 females were evaluated for growth, survival and external irregularities during lactation days 0, 4, 7, 14 and 21. F1 pups not selected for the adult generation were sacrificed and given a gross postmortem exam. Body weights and changes, food consumption, destation length and number of offspring were analyzed using ANOVA techniques followed by Dunnet's Test for parametric parameters and Kruskal-Willis test, Jonckheere or Mann-Whitney methods for nonparametric analysis. Mortality and pregnancy rates, fetal and mating indices and pup survival were analyzed using uncorrected Chi-square. Fisher's Exact test was used to statistically evaluate microscopic lesions. The level of significance was reported at both the 5% and 1% levels.

Result

Small, statistically significant decreases in body weights were observed in High Dose (1000 ppm) F0 males during the last three weeks on test (mean wts 94% of control) and in F1a dams of the same dose group (mean weights 93% of control) during lactation days 0-7. Food consumption was statistically reduced in 1000 ppm F0 females during the first 2 weeks of gestation. These minor deviations from the norm are not considered sufficiently severe to constitute an adverse effect. Thus, the NOAEL for

No Adverse reproductive effects were observed in adult rats or their offspring up to the highest dose tested, i.e. 1000 ppm, the reproductive

non-reproductive toxicity is considered 1000 ppm.

NOAEL for this study.

No treatment-related effects were noted in mating or fertility indices nor were any microscopic lesions attributable to treatment observed in reproductive organs (and other tissues) examined microscopically.

Test substance

Terminol 66; Daily average group mean dosages were calculated based on raw data for food consumption and body weight and were as follows:

Group (PPM): 30 100 300 1000

F0 males - 1.8, 6.1, 18.5 62.0 mg/kg/day F0 females - 2.5, 8.3, 42.2, 81.2 mg/kg/day

F1 males - 1.9, 6.1, 18.2, 63.1 mg/kg/day F1 females - 2.4, 8.1, 24.3, 80.6 mg/kg/day

Reliability : (2) valid with restrictions

22/28

Hematology, clinical chemistry, FOB and organ weights not conducted in this study, although all parameters were measured in subchronic study cited in this data package. Study itself sufficient to adequately judge fertility and reproductive indices.

Flag : Critical study for SIDS endpoint

5.11 ADDITIONAL REMARKS

24.07.2003 (19)

5.8.2	DEVELOPMENTAL TOXICITY/TERATOGENICITY
5.8.3	TOXICITY TO REPRODUCTION, OTHER STUDIES
5.9	SPECIFIC INVESTIGATIONS
5.10	EXPOSURE EXPERIENCE

6. Analyt. Meth. for Detection and Identification

ld 61788-32-7 **Date** 28.07.2003

- 6.1 ANALYTICAL METHODS
- 6.2 DETECTION AND IDENTIFICATION

7. Eff. Against Target Org. and Intended Uses

ld 61788-32-7 **Date** 28.07.2003

7.1	FUNCTION
7.2	EFFECTS ON ORGANISMS TO BE CONTROLLED
7.3	ORGANISMS TO BE PROTECTED
7.4	USER
7.5	RESISTANCE

8. Meas. Nec. to Prot. Man, Animals, Environment

ld 61788-32-7 **Date** 28.07.2003

8.1	METHODS HANDLING AND STORING
8.2	FIRE GUIDANCE
8.3	EMERGENCY MEASURES
8.4	POSSIB, OF RENDERING SUBST, HARMLESS
-	
8.5	WASTE MANAGEMENT
0.10	
8.6	SIDE-EFFECTS DETECTION
0.0	GDE ET EGIO DETEGNON
8.7	SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER
0.7	SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER
88	REACTIVITY TOWARDS CONTAINER MATERIAL
XX	REALTIVITY TOWARDS CONTAINER WATERIAL

9. References ld 61788-32-7 Date 28.07.2003

(1)	Solutia Technical report. THERMINOL 66. 03. 10-7 (5/03).
(2)	Solutia Study No. MO20020690. 1982. Vapor Pressure of MXP-2020 at Ambient Temperature.
(3)	Solutia Study no. MO-77-625. 1977. Comparison of Environmental Properties of CERECLOR 42 and SANTOSOL 340.
(4)	Solutia Study no. MO-95-248. 1995. Aqueous Solubility of SANTOTHERM 66.
(5)	Solutia Study No. MO20020691. 1982. Sunlight photolysis screening of MXP-2020.
(6)	EPISUITE v. 3.10, US Environmental Protection Agency (2000).
(7)	Solutia Study no. MO20020693. 1971. Biodegradation testing of Isopropylated Biphenyl (MIBP) and HB-40.
(8)	Solutia Study no. AB-79-135a. 1979. Acute toxicity of Therminol 66 to Fathead Minnows (Pimephales promelas).
(9)	Solutia Study no. AB-79-135b. 1979. Acute Toxicity of Therminol 66 to Rainbow Trout (Salmo gairdneri).
(10)	EPA's ECOSAR model (v. 0.99g). EPISUITE v. 3.10. US EPA (2000).
(11)	Solutia Study no. MO-96-204. 1996. The Toxicity of Therminol 66 (Partially Hydrogenated Terphenyls) to Daphnia magna.
(12)	Solutia Study no. AB-79-136. 1979. Acute Toxicity of Therminol 66 to Daphnia magna.
(13)	Solutia study no. BD19790137. 1979. Toxicity of Therminol 66 to the Freshwater Alga Selenastrum capricornutum.
(14)	Solutia study no. ML19790079. 1979. Acute Oral Toxicity of HB-40 Plasticizer in Rats.
(15)	Clark, CR, TC Marshall, BS Merickel, A Sanchez, DG Brownstein and CH Hobbs, 1979. Toxicological Assessment of Heat Transfer Fluids Proposed for Use in Solar Energy Applications. Toxicol. Appl. Pharmacol. 51:529-535.
(16)	Solutia study no. BD19840360. 1984. Three Month Oral Toxicity Feeding Study in Rats with THERMINOL 66.
(17)	Solutia Study no. DA78-184. 1978. Salmonella Mutagenicity Assay of HB 40.
(18)	Solutia Study no. SR-84-415. 1986. An Assessment of the Mutagenic Potential of THERMINOL 66 Utilizing the Acute In Vivo Rat Bone Marrow Cytogenetics Assay.
(19)	Solutia Study no. ML-90-135. 1991. Two Generation Reproduction Study of THERMINOL 66 Heat Transfer Fluid in the Diet of Albino Rats.

10. Summary and Evaluation

ld 61788-32-7 **Date** 28.07.2003

10.1	FND	POINT	SI	JMM	ARY

10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT